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NMR powder spectra in case of strong quadrupole interaction

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Abstract

We suggest the algorithm of straightforward numerical simulation of a powder NMR spectra in compounds with a strong quadrupole splittings. Results of our simulation exhibit a good fit of the experimental data even in case of moderate computing resources. It is shown that asymmetry parameter of the nuclear quadrupole interaction, quadrupole frequency and isotropic part of Knight shift can be evaluated from the powder NMR spectrum. The behavior of magnetic and quadrupole relaxation rates (the latter - at some assumption) over the spectra can be also simulated and allows one to determine the mechanism of nuclear spin lattice relaxation.

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Keywords

AsCu3, NMR, NQR, Powder, YBa2Cu3O7